

## Supplementary Figure S1.

id	Retention time (min)	m/z(-) detected	m/z(-) expected	elemental formula	Mass Error (ppm)	PUTATIVE IDENTIFICATION	METABOLITE CLASS	minimum metabolite level										maximum metabolite level										
								p[1]	p[2]	WINE EXTRACT	CS-1	CS-3	CS-5	C10-1	C10-3	C10-5	C20-1	C20-3	C20-5	TS-1	TS-3	TS-5	T10-1	T10-3	T10-5	T20-1	T20-3	T20-5
1	8.80483333	955,24949	955,259	C56H42O12	-4.872704551	resveratrol tetramer	stilbenes and viciiflorins	0.502241	0.155021	5.184										1.763	5.902	6.979	2.564	7.499	12.574	1.084	2.501	5.715
2	7.43068333	499,13796	499,139	C28H22O6	-2.09200049	epigallocatechin gallate (formic adduct)	stilbenes and viciiflorins	0.271712	0.102033	3.091	34	35	84	33	34	31	35	36	34	406	1.844	1.032	6.97	2.211	3.77	1.192	1.679	
3	9.27643333	951,25947	951,265	C56H42O12	-8.332480769	resveratrol tetramer (formic adduct)	stilbenes and viciiflorins	0.196106	0.066088	474										243	983	1.608	286	1.089	1.808	49	330	417
4	8.806	447,0702					stilbenes and viciiflorins	0.195239	0.051159	788										474	1.332	2.044	249	936	1.532	211	279	941
5	8.8176	725,15854					stilbenes and viciiflorins	0.17897	0.045482	409	2	10	21	0	0	0	0	0	0	244	894	1.434	249	870	1.509	63	303	473
6	8.49268333	447,07018					stilbenes and viciiflorins	0.126759	0.043139	9	0	0	0	0	0	0	0	0	0	147	584	328	113	403	448	77	293	440
7	12.7159	571,28859					stilbenes and viciiflorins	0.126001	0.056506	292	0	0	12	74	0	0	0	0	0	30	250	491	150	844	1.443			
8	8.0048	499,13798	499,139	C28H22O6	-2.036625798	epigallocatechin (formic adduct)	stilbenes and viciiflorins	0.111379	0.045331	465										44	316	505	96	370	411	55	194	333
9	8.55566667	951,25707	951,265	C56H42O12	-8.332480769	resveratrol tetramer (formic adduct)	stilbenes and viciiflorins	0.102039	0.042238	370										46	210	436	60	311	548	13	111	209
10	7.43068333	499,13796					stilbenes and viciiflorins	0.131431	0.039229	423	0	0	0	2	1	0	2	4	0	65	244	433	96	286	88	49	160	243
11	8.43216667	499,13813	499,139	C28H22O6	-1.747786112	epigallocatechin (formic adduct)	stilbenes and viciiflorins	0.100677	0.045942	526										54	240	437	82	287	313	47	211	333
12	6.06471667	575,11891	575,118	C30H26O13	-1.901901376	prodelphinidin Pp-P (M-H2O adduct)	flavan-3-ols and	0.099533	0.033693	1.493									45	272	439	53	281	313	39	39	127	
13	9.27643333	498,13551					flavan-3-ols and	0.097449	0.034244	88									63	232	434	54	274	471	12	95	150	
14	6.52393	863,17119	863,182	C45H38O19	-12.51851385	prodelphinidin Pp-P (M-H2O adduct)	flavan-3-ols and	0.097363	0.041932	1.264									25	184	345	62	325	371	5	74	171	
15	7.43068333	499,13796					flavan-3-ols and	0.094382	0.034849	292									46	222	368	71	241	474	25	122	191	
16	8.88048333	1023,1894					flavan-3-ols and	0.091681	0.038951	158									22	180	348	59	243	432	12	88	143	
17	5.46155	865,19278	865,197	C45H38O19	-4.872385232	prodelphinidin P3 type	flavan-3-ols and	0.091151	0.067908	26,740	4	3	2	0	2	4	0	0	0	12	129	205	95	380	443	92	377	636
18	9.02485	587,0805					flavan-3-ols and	0.090921	0.024854	108									0	37	233	421	60	227	394	13	40	94
19	8.5346	725,15799					flavan-3-ols and	0.090679	0.037119	188									0	39	189	342	55	235	404	4	116	128
20	8.43283	865,19361					flavan-3-ols and	0.089587	0.031517	405									0	79	327	343	50	193	333	2	4	24
21	5.38818333	863,17565	863,182	C45H38O19	-7.161673913	prodelphinidin A-P3 type	flavan-3-ols and	0.089009	0.029431	2,531									0	43	184	302	54	224	434	2	19	103
22	8.72326667	906,25731					flavan-3-ols and	0.082381	0.031917	36									0	26	155	291	36	184	302	6	54	112
23	7.74271	435,10891	435,107	C24H20O8	-0.209625504	Epigallocatechin 3-O-succinate	flavan-3-ols and	0.081552	0.065701	2,379									0	47	188	311	64	252	431	137	503	816
24	7.19198333	517,14722	517,134	C25H20O12	25.57274848	vitamin B	flavan-3-ols and	0.079281	0.03715	1,279									0	25	146	253	60	197	314	26	127	214
25	8.13868333	725,15803					flavan-3-ols and	0.079172	0.035812	1,361									0	20	151	272	28	165	304	11	45	145
26	8.63941667	545,17849					flavan-3-ols and	0.077339	0.038391	379									0	31	147	239	46	191	302	45	146	248
27	8.37783333	725,15731					flavan-3-ols and	0.076481	0.030042	133									0	30	148	238	28	174	301	9	74	121
28	6.03283333	863,17268	863,182	C45H38O19	-10.80176721	prodelphinidin Pp-P (M-H2O adduct)	flavan-3-ols and	0.075072	0.027652	493	0	2	3	0	0	3	0	0	0	10	138	234	46	179	308	4	40	79
29	8.60821667	577,13407	577,134	C30H26O13	0.122688275	prodelphinidin P2 type	flavan-3-ols and	0.073983	0.041906	64,006									0	24	95	147	65	214	372	45	147	248
30	6.52393	575,11877	575,118	C30H26O13	-2.145197516	prodelphinidin P2 type	flavan-3-ols and	0.072564	0.031939	339									0	29	176	264	38	131	242	13	25	44
31	11.01496667	498,13796					flavan-3-ols and	0.069679	0.031939	137	0	15	13	24	14	25	24	15	0	49	120	177	50	174	242	27	105	139
32	6.68071667	735,13361					flavan-3-ols and	0.06931	0.029235	137	0	0	0	2	0	0	0	0	0	19	120	177	50	174	242	27	105	139
33	7.69035	529,14825					flavan-3-ols and	0.064894	0.025673	142									0	24	103	186	27	121	227	14	63	105
34	6.90888333	575,11734	575,118	C30H26O13	-0.00461985	prodelphinidin P2 type	flavan-3-ols and	0.063818	0.030486	127									0	7	70	146	25	123	208	12	57	98
35	7.59883333	607,14288					flavan-3-ols and	0.061346	0.023597	426									0	30	138	208	20	94	147	25	70	149
36	8.806	603,07772					flavan-3-ols and	0.061291	0.030461	86									0	11	46	116	36	121	202	15	44	114
37	7.43068333	265,04873					flavan-3-ols and	0.060954	0.024645	148									0	21	90	150	26	109	184	9	56	89
38	9.07726667	645,17331					flavan-3-ols and	0.060317	0.024477	15									0	15	114	195	19	82	135	11	65	109
39	6.94773333	575,11759	575,118	C30H26O13	-0.718927858	prodelphinidin P2 type	flavan-3-ols and	0.059357	0.028533	385									0	14	48	116	26	123	208	13	68	99
40	9.37886667	294,06239					flavan-3-ols and	0.058664	0.022964	423	40	40	46	38	37	32	34	34	41	38	148	248	63	119	208	57	115	164
41	5.14856667	300,99161	300,998	C14H16O8	-1.96957317	ellagic acid	stilbenes and viciiflorins	0.058006	0.049726	5,473	14	7	15	19	19	0	0	0	0	42	144	238	52	119	208	57	115	164
42	9.30306667	499,13888	499,139	C28H22O6	-0.243853338	epigallocatechin (formic adduct)	stilbenes and viciiflorins	0.057683	0.035312	1,931	0	0	0	0	0	0	0	0	0	13	85	148	21	102	148	32	119	208
43	7.73226667	435,11335					stilbenes and viciiflorins	0.056449	0.030944	128	18	71	238	22	46	268	19	49	146	18	71	238	22	46	268	19	49	146
44	6.12761667	739,16218					stilbenes and viciiflorins	0.054443	0.035517	2,379	0	0	0	0	0	0	0	0	0	3	26	109	9	115	188	13	83	136
45	6.3687	477,06854	477,066	C21H18O13	1.138245939	quercetin-O-glucuronide	flavonoids	0.05402	0.009569	10,244									0	29	129	234	14	63	114	28	27	44
46	6.88235	507,11322	507,113	C21H22O11	0.442677737	rhovanetin-3-O-glucuronide (formic adduct)	flavonoids	0.053763	0.027579	19,171									0	25	82	144	20	64	104	23	27	44
47	8.90955	227,07034	227,070	C14H12O3	1.500488281	resveratrol	stilbenes and viciiflorins	0.053388	0.052548	1,825	49	81	84	47	53	54	89	46	48	65	131	170	87	193	282	163	388	419
48	6.46005	723,16548					stilbenes and viciiflorins	0.051719	0.034564	1,805	1	6	0	2	0	2	3	0	0	44	74	138	107	196	114	81	138	138
49	6.69125	723,16475					stilbenes and viciiflor																					